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Publons / Web Of Science ResearcherID: ABB-3380-2021

ScopusID: 55622925500

Yoksis Araştırmacı ID: 157331

Eğitim Bilgileri

Doktora, Ondokuz Mayıs Üniversitesi, Lisansüstü Eğitim Enstitüsü, Kimya Anabilim Dalı, Türkiye 2014 - 2019

Yüksek Lisans, Ondokuz Mayıs Üniversitesi, Fen Bilimleri Enstitüsü, Kimya (YI) (Tezli), Türkiye 2011 - 2014

Lisans, Süleyman Demirel Üniversitesi, Fen-Edebiyat Fakültesi, Kimya Bölümü, Türkiye 2006 - 2010

Yaptığı Tezler

Doktora, Bir seri makrogol bağlı simetrik ve asimetric yapıli ftalosiyanın bileşiklerinin sentezi ve karakterizasyonu, Ondokuz Mayıs Üniversitesi, Kimya (Dr), 2019

Yüksek Lisans, Makromoleküler ağ örgülü ftalosiyanın polimerik ftalosiyanın bileşiklerinin sentezi ve karakterizasyonu, Ondokuz Mayıs Üniversitesi, 2014

Araştırma Alanları

Temel Bilimler

Akademik Unvanlar / Görevler

Araştırma Görevlisi Dr., Ondokuz Mayıs Üniversitesi, Fen Fakültesi, Kimya Bölümü, 2011 - Devam Ediyor

SCI, SSCI ve AHCI İndekslerine Giren Dergilerde Yayımlanan Makaleler

- I. A Schiff Base with Polymorphic Structure ($Z'=2$): Investigations with Computational Techniques and in Silico Predictions
Şahin S., Can N. N.
POLYCYCLIC AROMATIC COMPOUNDS, cilt.43, sa.10, ss.9269-9294, 2023 (SCI-Expanded)
- II. A New Molecular Structure and Computational Analyses: DFT Studies, NLO Properties, ADMET

Predictions, Biological Targets, and Docking Experiments

Şahin S.

Polycyclic Aromatic Compounds, 2023 (SCI-Expanded)

- III. **A single-molecule with multiple investigations: Synthesis, characterization, computational methods, inhibitory activity against Alzheimer's disease, toxicity, and ADME studies**
Şahin S.
COMPUTERS IN BIOLOGY AND MEDICINE, cilt.146, 2022 (SCI-Expanded)
- IV. **(E)-N-(3-chlorophenyl)-1-(5-nitro-2-(piperidin-1-yl)phenyl)methanimine: X-Ray, DFT, ADMET, Boiled-Egg Model, Druggability, Bioavailability, and Human Cyclophilin D (CypD) Inhibitory Activity**
Şahin S., DEGE N.
JOURNAL OF MOLECULAR STRUCTURE, cilt.1250, 2022 (SCI-Expanded)
- V. **Synthesis, characterization, computational analyses, in silico ADMET studies, and inhibitory action against SARS-CoV-2 main protease (Mpro) of a Schiff base**
Şahin S., DEGE N.
TURKISH JOURNAL OF CHEMISTRY, cilt.46, sa.5, ss.1548-1572, 2022 (SCI-Expanded)
- VI. **Synthesis, characterization, X-ray, HOMO-LUMO, MEP, FT-IR, NLO, Hirshfeld surface, ADMET, boiled-egg model properties and molecular docking studies with human cyclophilin D (CypD) of a Schiff base compound: (E)-1-(5-nitro-2-(piperidin-1-yl)phenyl)-N-(3-nitrophenyl) methanimine**
Şahin S., DEGE N.
POLYHEDRON, cilt.205, 2021 (SCI-Expanded)
- VII. **A newly synthesized small molecule: the evaluation against Alzheimer's Disease by in silico drug design and computational structure analysis methods**
Şahin S., DEGE N.
JOURNAL OF MOLECULAR STRUCTURE, cilt.1236, 2021 (SCI-Expanded)
- VIII. **A3B type unsymmetrical and amphiphilic phthalocyanines: Synthesis, characterization, thermal stability and aggregation studies**
Şahin S., Ağar E.
SPECTROCHIMICA ACTA PART A-MOLECULAR AND BIOMOLECULAR SPECTROSCOPY, cilt.227, 2020 (SCI-Expanded)
- IX. **Synthesis, spectroscopic properties, thermal properties and aggregation behaviors of macrogol-substituted phthalocyanines**
Şahin S., Ağar E.
JOURNAL OF MOLECULAR STRUCTURE, cilt.1187, ss.121-131, 2019 (SCI-Expanded)
- X. **The Crystallographic, Spectroscopic and Theoretical Studies on (E)-2-(((4-fluorophenyl)imino)methyl)-4-nitrophenol and (E)-2-(((3-fluorophenyl)imino)methyl)-4-nitrophenol Compounds**
Demirtas G., DEGE N., Ağar E., Şahin S.
IRANIAN JOURNAL OF CHEMISTRY & CHEMICAL ENGINEERING-INTERNATIONAL ENGLISH EDITION, cilt.37, sa.5, ss.55-65, 2018 (SCI-Expanded)
- XI. **Crystal Structure of 2-((E)-(5-Bromo-2-hydroxybenzylidene)hydrazono)-1,2-diphenylethanone(1)**
Kaynar N. K., Yavuz M., TANAK H., Şahin S., Buyukgungor O., Ağar E.
CRYSTALLOGRAPHY REPORTS, cilt.63, sa.3, ss.375-378, 2018 (SCI-Expanded)
- XII. **Molecular and Crystal Structure of 2-((E)-[(5-Chloro-2-methoxyphenyl)imino]methyl)-4-nitrophenol(1)**
Kaynar N. K., Ağar E., TANAK H., Şahin S., Buyukgungor O., Yavuz M.
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- XIII. **Crystal structure of (E)-4-nitro-2-((2-phenoxy-phenylimino)methyl)phenol, C₁₉H₁₄N₂O₄**
Köysal Y., Bülbül H., Kantar E. N., Coskun E., Şahin S., DEGE N.
ZEITSCHRIFT FÜR KRISTALLOGRAPHIE-NEW CRYSTAL STRUCTURES, cilt.232, sa.1, ss.9-10, 2017 (SCI-Expanded)
- XIV. **Molecular and crystal structure of 2-((E)-[(4-Methylphenyl)imino]methyl)-4-nitrophenol: A redetermination**

Kaynar N. K., TANAK H., Şahin S., DEGE N., Ağar E., Yavuz M.
CRYSTALLOGRAPHY REPORTS, cilt.61, sa.2, ss.239-242, 2016 (SCI-Expanded)

- XV. **Crystal structure and spectroscopic characterization of (E)-2-(((4-bromo-2-(trifluoromethoxy)phenyl)imino)methyl)-4-nitrophenol: A combined experimental and computational study**
Tamer O., DEGE N., Demirtas G., AVCI D., ATALAY Y., Macit M., Şahin S.
JOURNAL OF MOLECULAR STRUCTURE, cilt.1063, ss.295-306, 2014 (SCI-Expanded)

Diğer Dergilerde Yayınlanan Makaleler

- I. **Crystal structure of 2-[[2-methoxy-5-(trifluoromethyl)phenyl]iminomethyl]-4-nitrophenol**
Karadayı N., Şahin S., Köysal Y., Coskun E., Buyukgungor O.
ACTA CRYSTALLOGRAPHICA SECTION E-CRYSTALLOGRAPHIC COMMUNICATIONS, cilt.71, 2015 (ESCI)
- II. **2-[[3-Chloro-4-(4-chlorophenoxy)phenyl]iminomethyl]-4-nitrophenol**
Karadayı N., Köysal Y., Şahin S., Coskun E., Buyukgungor O.
ACTA CRYSTALLOGRAPHICA SECTION E-CRYSTALLOGRAPHIC COMMUNICATIONS, cilt.69, 2013 (ESCI)

Hakemli Kongre / Sempozyum Bildiri Kitaplarında Yer Alan Yayınlar

- I. **IN SILICO ASSESSMENT OF TYPE 2 DIABETES MELLITUS DRUGS AGAINST AMYLOID-B AND TAU AGGREGATION-FORMING SEGMENTS (KLVFFA, VQIVYK, GGVVIA, VQIINK) FOR ALZHEIMER'S DISEASE**
ŞAHİN S.
Materials, Method, and Technologies 2022, 24th International conference, 19-22 August, Burgas, BULGARIA, Burgas, Bulgaristan, 19 - 22 Ağustos 2022, ss.351-362
- II. **Dual-targeting of β -amyloid and Tau Aggregation against Alzheimer's Disease with the Approved Trifluorinated Drugs**
ŞAHİN S.
Global Congress on Pharmaceutical Sciences and Clinical Research 2022, Japonya, 20 - 22 Temmuz 2022, ss.117-125
- III. **Sentezlenen Schiff Bazı İçeren Bileşiğin Yapısal ve Spektroskopik Özelliklerinin Deneysel ve Teorik İncelenmesi**
KARAKURT T., AĞAR E., ŞAHİN S., YILDIZ Ş., PARLAK C.
III. International Scientific and Vocational Studies Congress - Science and Health, Nevşehir, Türkiye, 27 - 30 Haziran 2019, ss.174-182
- IV. **Computational Investigations and Experimental of (E)-2-((2,4-dichlorophenylimino)methyl)-4-nitrophenol**
KARADAYI N., ŞAHİN S., AĞAR E., BÜYÜKGÜNGÖR O.
International Computational Science Congress(CSC2018), 26 - 28 Ekim 2018
- V. **Computational and Experimental Investigations of (E)-2-((2,4-dichlorophenylimino)methyl)-4-nitrophenol**
KARADAYI N., ŞAHİN S., AĞAR E., BÜYÜKGÜNGÖR O.
CSC2018 - Computational Science Congress, Amasya, Türkiye, 26 - 21 Ekim 2018, ss.104-111
- VI. **An Investigation on Aggregation Status of Macrogol-Bound Zinc Phthalocyanine in Different Solvents**
ŞAHİN S., AĞAR E.
6th International BAU Drug Design Congress, 13 - 15 Aralık 2018
- VII. **An Investigation about Aggregation Properties of Copper Phthalocyanine Bearing TEG**
ŞAHİN S., AĞAR E.
4 th Organic Chemistry Congress with International Participation, Antalya, Türkiye, 4 - 07 Ekim 2018

- VIII. **Investigating of Spectroscopic Properties and Synthesis of Phthalocyanines Substituted with 2,2'-xx-Methylenebis(4-chlorophenoxy)**
ŞAHİN S., ERŞAHİN F., AĞAR E.
Tenth International Conference on Porphyrines and Phthalocyanines, Munich, Almanya, 1 - 06 Temmuz 2018
- IX. **Investigating of Spectroscopic Properties and Synthesis of Phthalocyanine Containing Some Aza Group**
ŞAHİN S., ERŞAHİN F., AĞAR E.
Tenth International Conference Porphyrines and Phthalocyanines, Munich, Almanya, 1 - 06 Temmuz 2018
- X. **X-ray crystallographic and computational studies of (E)-2-(((4-bromophenyl)imino)methyl) -4,5-difluorophenol**
ATALAY Ş., DURSUN M. E., BÜLBÜL H., AĞAR E., ŞAHİN S.
Turkish Physical Society 33rd International Physics Congress, BODRUM / MUĞLA, Türkiye, 6 - 10 Eylül 2017
- XI. **THE THEORETICAL AND CRYSTALLOGRAPHIC STUDIES ON (E)-2-(((4-BROMO-2-(TRIFLUOROMETHOXY)PHENYL)IMINO)METHYL)-4-NITROPHENOL**
DEMİRTAŞ G., TAMER Ö., DEGE N., AVCI D., ATALAY Y., MACİT M., ŞAHİN S.
TURKISH PHYSICAL SOCIETY 33RD INTERNATIONAL PHYSICS CONGRESS, 6 - 10 Eylül 2017
- XII. **Synthesis and Characterization of Some Polymeric Phthalocyanine Compounds**
ŞAHİN S., Taşçı C., TOPCU Y., AĞAR E.
Eight International Conference on Porphyrins and Phthalocyanines ICPP-8, İstanbul, Türkiye, 22 - 27 Haziran 2014, ss.680
- XIII. **(E)-2-((4-Etilfenilimino)metil)-4-nitrofenol Bileşiğinin Deneysel ve Hesaplamalı Yöntemlerle İncelenmesi**
ALPASLAN G., AĞAR E., ŞAHİN S., GÖKCE H., CEYLAN Ü., ÖZDEMİR N.
21. Yoğun Madde Fiziği Ankara Toplantısı, Ankara, Türkiye, 25 Aralık 2015, ss.19
- XIV. **Synthesis of Peripheral-Substituted Metal and Metal-Free Network Polymeric Phthalocyanine Compounds**
ŞAHİN S., AĞAR E.
International Conference on Porphyrins and Phthalocyanines, 22 - 27 Haziran 2014
- XV. **Synthesis and Characterization of Some Polymeric Phthalocyanine Compounds**
ŞAHİN S., TAŞCI C., TOPCU Y., AĞAR E.
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